

Reax-force field as described in Sanz-Navarro et al. (Molecular Dynamics Simulations of the Interactions between Platinum Clusters and Carbon Platelets). For parameter names see the supplement of Nielson et al. (JPC-A 2005)

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39      ! Number of general parameters
50.0000 !p(boc1)
9.5469  !p(boc2)
26.5405 !p(coa2)
4.6420 !Triple bond stabilisation parameter
7.2181 !Triple bond stabilisation parameter
0.0000 !kc2
1.0588 !p(ovun6)
9.0000 !Triple bond stabilisation parameter
11.2373 !p(ovun7)
13.3056 !p(ovun8)
-15.0000 !Triple bond stabilization energy
0.0000 !Lower Taper-radius (swa)
10.0000 !Upper Taper-radius (swb)
2.8793 !Not used
33.8667 !p(val7)
6.0891 !p(lp1)
1.0563 !p(val9)
2.0384 !p(val10)
6.1431 !Not used
6.9290 !p(pen2)
0.3989 !p(pen3)
3.9954 !p(pen4)
-2.4837 !Not used
5.7796 !p(tor2)
10.0000 !p(tor3)
1.9487 !p(tor4)
-1.2327 !Not used
2.1645 !p(cot22)
1.5591 !p(vdW1)
0.1000 !Cutoff for bond order (*100) (cutoff)
2.1365 !p(coa4)
0.6991 !p(ovun4)
1.2593 !p(ovun3)
1.8512 !p(val8)
0.5000 !Not used
20.0000 !Not used
5.0000 !Not used
0.0000 !Not used
2.6962 !p(coa3)
4      !Nr of atoms. atomID;ro(sigma);Val;atom mass;RvdW;Dij;gamma;ro(pi);Val(e)
      alfa;gamma(w);Val(angle);p(ovun5);n.u.;chiEEM;etaEEM;n.u.
      ro(pipi);p(lp2);Heat increment;p(boc4);p(boc3);p(boc5);n.u.;n.u.
      p(ovun2);p(val3);n.u.;Val(boc);p(val5);n.u.;n.u.;n.u.
C      1.3644 4.0000 12.0000 1.9803 0.1720 0.8712 1.2395 4.0000
      9.4734 2.1241 4.0000 31.8793 79.5548 5.7254 6.9235 0.0000
      1.2636 0.0000 -0.0537 5.7133 33.5629 11.9957 0.8563 0.0000
      -2.8983 4.7820 1.0564 4.0000 2.9663 0.0000 0.0000 0.0000
H      0.6853 1.0000 1.0080 1.3588 0.0622 0.9895 -0.1000 1.0000
      9.3992 5.0518 1.0000 0.0000 121.1250 5.7873 7.4100 1.0000
      -0.1000 0.0000 -0.1609 2.5817 4.1491 1.2385 1.0698 0.0000
      -15.7683 2.1488 1.0338 1.0000 2.8793 0.0000 0.0000 0.0000
Pt     1.9318 2.0000 195.0800 2.0163 0.2920 0.6396 -1.0000 2.0000

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		12.3885	6.1726	2.0000	0.0000	0.0000	6.3388	5.7617	0.0000
		-1.0000	0.0000	143.1770	22.5697	7.4147	0.1552	0.8563	0.0000
		-7.3154	1.8009	1.0338	5.0000	2.5791	0.0000	0.0000	0.0000
X		-0.1000	2.0000	1.0080	2.0000	0.0000	1.0000	-0.1000	6.0000
		10.0000	2.5000	4.0000	0.0000	0.0000	8.5000	1.5000	0.0000
		-0.1000	0.0000	-2.3700	8.7410	13.3640	0.6690	0.9745	0.0000
		-11.0000	2.7466	1.0338	6.2998	2.8793	0.0000	0.0000	0.0000

6 !Nr of bonds.

at1;at2;De(sigma);De(pi);De(pipi);p(be1);p(bo5);13corr;n.u.;p(bo6);p(ovun1)

p(be2);p(bo3);p(bo4);n.u.;p(bo1);p(bo2)

1	1	139.8093	110.6913	77.2102	0.2737	-0.7584	1.0000	38.4226	0.3288
		0.1235	-0.2010	8.6973	1.0000	-0.1042	6.1688	1.0000	0.0000
1	2	160.3488	0.0000	0.0000	-0.4750	0.0000	1.0000	6.0000	0.7128
		5.9163	1.0000	0.0000	1.0000	-0.0440	5.6835	0.0000	0.0000
2	2	167.4522	0.0000	0.0000	-0.3573	0.0000	1.0000	6.0000	0.7489
		9.6471	1.0000	0.0000	1.0000	-0.0169	5.9140	0.0000	0.0000
1	3	141.0293	0.0000	0.0000	0.0368	-0.2000	1.0000	16.0000	0.4061
		0.1200	-0.2000	15.0000	1.0000	-0.1400	6.7008	1.0000	0.0000
2	3	160.2066	0.0000	0.0000	-0.2235	0.0000	1.0000	6.0000	0.3378
		17.4884	1.0000	0.0000	1.0000	-0.0531	10.4657	0.0000	0.0000
3	3	98.9857	0.0000	0.0000	-0.2768	-0.2000	0.0000	16.0000	0.2903
		0.7541	-0.2000	15.0000	1.0000	-0.0931	4.7088	0.0000	0.0000

3 ! Nr of off-diagonal terms.

at1;at2;Dij;RvdW;alfa;ro(sigma);ro(pi);ro(pipi)

1	2	0.0435	1.6842	10.3839	1.0687	-1.0000	-1.0000
1	3	0.0800	1.5534	13.5470	1.7857	-1.0000	-1.0000
2	3	0.0382	1.8337	11.7280	1.6046	-1.0000	-1.0000

17 ! Nr of angles.

at1;at2;at3;Thetao,o;p(val1);p(val2);p(coal);p(val7);p(pen1);p(val4)

1	1	1	75.8304	33.9168	0.8043	0.0000	0.1780	10.5736	1.0400
1	1	2	69.6421	9.2578	3.6521	0.0000	0.0058	0.0000	1.0400
2	1	2	75.4958	14.5436	2.7438	0.0000	0.0127	0.0000	1.0400
1	2	2	0.0000	0.0000	6.0000	0.0000	0.0000	0.0000	1.0400
1	2	1	0.0000	3.4110	7.7350	0.0000	0.0000	0.0000	1.0400
2	2	2	0.0000	27.9213	5.8635	0.0000	0.0000	0.0000	1.0400
1	1	3	46.8437	17.7937	6.9466	0.0000	0.1276	0.0000	2.8158
3	1	3	40.9228	18.5964	6.8639	0.0000	0.1000	0.0000	1.0587
1	3	3	37.4285	1.0000	1.0136	0.0000	0.5801	0.0000	2.5988
1	3	1	37.5291	7.4679	1.6697	0.0000	1.0031	0.0000	2.2937
2	1	3	33.8363	11.6424	2.9259	0.0000	0.9059	0.0000	3.0000
1	3	2	86.0878	1.3988	0.2231	0.5000	1.3748	0.0000	1.5790
1	2	3	0.0000	2.3184	0.5764	0.0000	0.1752	0.0000	1.0618
2	3	2	57.3916	22.7625	0.8385	0.0000	1.9462	0.0000	1.1000
2	2	3	0.0000	3.3503	1.6083	0.0000	0.3066	0.0000	1.5060
3	2	3	0.0000	3.8954	2.7531	0.0000	0.6569	0.0000	2.9482
2	3	3	88.3592	5.8119	4.6578	0.0000	1.1634	0.0000	1.6383

6 ! Nr of torsions. at1;at2;at3;at4;;V1;V2;V3;p(tor1);p(cot1);n.u;n.u.

1	1	1	0.0000	38.9174	0.3649	-8.2931	-2.0127	0.0000	0.0000
1	1	1	2	0.0000	49.1001	0.2713	-8.5284	-1.5309	0.0000
2	1	1	2	0.0000	34.0265	0.3804	-6.3917	-0.9965	0.0000
0	1	2	0	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0	2	2	0	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0	1	1	0	0.0000	0.6675	0.0000	-8.2352	0.0000	0.0000

0 ! Nr of hydrogen bonds. at1;at2;at3;r(hb);p(hb1);p(hb2);p(hb3)